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Title: w19_OMEC Scientific Highlight

Author(s): Zelenay, Piotr
Yin, Xi
Holby, Edward F.

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w19_OMEC Scientific Highlight

Scientific Achievement

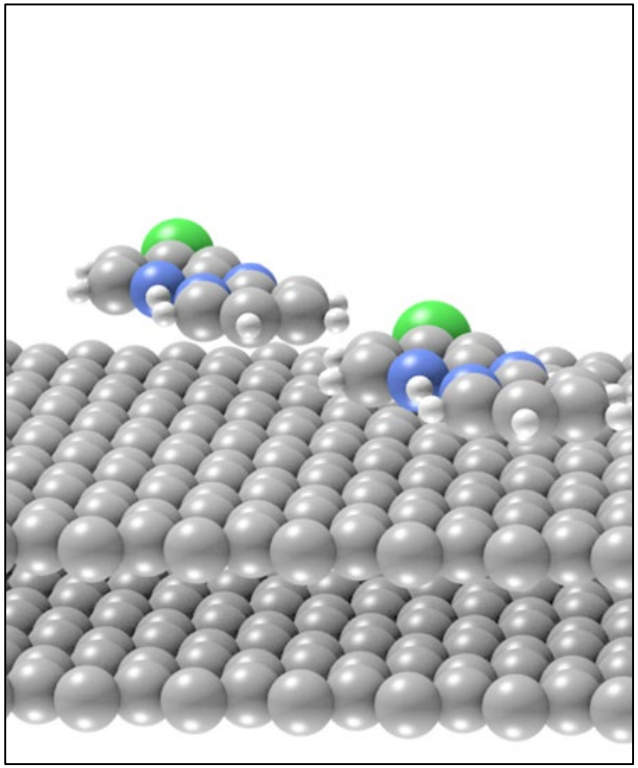
- Revealed the effect of graphite substrate on H binding / hydrogen evolution reaction (HER) activity of organic molecular electrocatalysts (OMECs)
- Demonstrated the effect of molecular modification on calculated HER activity descriptor

Significance and Impact

- Understanding of HER processes is important for discovering low-cost OMECs for hydrogen production and energy application
- Design of OMEC structures remains challenging due to the unexplored redox properties of organic molecules
- Density functional theory (DFT) has been proposed to provide needed insights into HER activity for improved materials design

Research Details

- DFT calculations on the binding energy of HER intermediates are used for predicting reduction potentials and calculated H adsorption energy as activity descriptor
- LANL Institutional Computing (IC) resources are essential for successful project execution given the size of structures involved in modeling molecule-support interaction



Adsorption of H atom at pyridyl-N site in chlorine-substituted DPA molecule on graphite support surface.